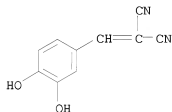


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L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 118409-57-7 REGISTRY
ED Entered STN: 13 Jan 1989
CN Propanedinitrile, 2-[(3,4-dihydroxyphenyl)methylene]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Propanedinitrile, [(3,4-dihydroxyphenyl)methylene]- (9CI)
OTHER NAMES:
CN (3,4-Dihydroxybenzylidene)malononitrile
CN 2-(3,4-Dihydroxybenzylidene)malononitrile
CN AG 18
CN AG 18 (pharmaceutical)
CN RG 50810
CN RG 50858
CN TX 825
CN Tyrphostin 23
CN Tyrphostin A 23
CN Tyrphostin AG 18
DR 163063-13-6, 155070-88-5
MF C10 H6 N2 O2
CI COM
SR CA
LC STN Files: ADISINSIGHT, AGRICOLA, BEILSTEIN*, BIOSIS, BIOTECHNO, CA,
CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, DDFU, DRUGU, EMBASE,
MEDLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

120 REFERENCES IN FILE CA (1907 TO DATE)
121 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d prop

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	NOTE
=====+=====+=====		
Melting Point (MP)	225 deg C	(1) IC

(1) Gazit, Aviv; Journal of Medicinal Chemistry 1989 V32(10) P2344-52
CAPLUS

Experimental Property Tags (ETAG)

PROPERTY		NOTE
Mass Spectra	(1)	IC
NMR Spectra	(1)	IC
Proton NMR Spectra	(1)	IC

(1) Gazit, Aviv; Journal of Medicinal Chemistry 1989 V32(10) P2344-52
CAPLUS

Predicted Properties (PPROP)

PROPERTY (CODE)		VALUE		CONDITION		NOTE
Bioconc. Factor (BCF)		3.30		pH 1 25 deg C		(1)
Bioconc. Factor (BCF)		3.30		pH 2 25 deg C		(1)
Bioconc. Factor (BCF)		3.30		pH 3 25 deg C		(1)
Bioconc. Factor (BCF)		3.30		pH 4 25 deg C		(1)
Bioconc. Factor (BCF)		3.28		pH 5 25 deg C		(1)
Bioconc. Factor (BCF)		3.13		pH 6 25 deg C		(1)
Bioconc. Factor (BCF)		2.13		pH 7 25 deg C		(1)
Bioconc. Factor (BCF)		1.0		pH 8 25 deg C		(1)
Bioconc. Factor (BCF)		1.0		pH 9 25 deg C		(1)
Bioconc. Factor (BCF)		1.0		pH 10 25 deg C		(1)
Boiling Point (BP)		421.1+/-45.0 deg C		760 Torr		(1)
Density (DEN)		1.428+/-0.06 g/cm**3		20 deg C		(1)
				760 Torr		
Enthalpy of Vap. (HVAP)		70.13+/-3.0 kJ/mol		760 Torr		(1)
Flash Point (FP)		208.5+/-28.7 deg C				(1)
Freely Rotatable Bonds (FRB)		3				(1)
H acceptors (HAC)		4				(1)
H donors (HD)		2				(1)
Hydrogen Donors/Acceptors Sum (HDAS)		6				(1)
Koc (KOC)		81.80		pH 1 25 deg C		(1)
Koc (KOC)		81.80		pH 2 25 deg C		(1)
Koc (KOC)		81.80		pH 3 25 deg C		(1)
Koc (KOC)		81.75		pH 4 25 deg C		(1)
Koc (KOC)		81.35		pH 5 25 deg C		(1)
Koc (KOC)		77.51		pH 6 25 deg C		(1)
Koc (KOC)		52.68		pH 7 25 deg C		(1)
Koc (KOC)		12.56		pH 8 25 deg C		(1)
Koc (KOC)		1.50		pH 9 25 deg C		(1)
Koc (KOC)		1.0		pH 10 25 deg C		(1)
LOGD (LOGD)		0.99		pH 1 25 deg C		(1)
LOGD (LOGD)		0.99		pH 2 25 deg C		(1)
LOGD (LOGD)		0.99		pH 3 25 deg C		(1)
LOGD (LOGD)		0.99		pH 4 25 deg C		(1)
LOGD (LOGD)		0.98		pH 5 25 deg C		(1)
LOGD (LOGD)		0.96		pH 6 25 deg C		(1)
LOGD (LOGD)		0.79		pH 7 25 deg C		(1)
LOGD (LOGD)		0.17		pH 8 25 deg C		(1)
LOGD (LOGD)		-0.75		pH 9 25 deg C		(1)

LOGD (LOGD)	-1.63	pH 10 25 deg C	(1)
LOGP (LOGP)	0.985+/-0.750	25 deg C	(1)
Mass Intrinsic Solubility	0.41 g/L	25 deg C	(1)
(ISLB.MASS)			
Mass Solubility (SLB.MASS)	0.41 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.41 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.41 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.41 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.41 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.43 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	2.6 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	22 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	170 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.41 g/L	Unbuffered Water	(1)
		pH 4.96	
		25 deg C	
Molar Intrinsic Solubility	0.0022 mol/L	25 deg C	(1)
(ISLB.MOL)			
Molar Solubility (SLB.MOL)	0.0022 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0022 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0022 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0022 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0022 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0023 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0034 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.014 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.12 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.92 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0022 mol/L	Unbuffered Water	(1)
		pH 4.96	
		25 deg C	
Molar Volume (MVOL)	130.3+/-3.0 cm**3/mol	20 deg C	(1)
		760 Torr	
Molecular Weight (MW)	186.17		(1)
PKA (PKA)	7.24+/-0.18	Most Acidic	(1)
		25 deg C	
Polar Surface Area (PSA)	88.04 A**2		(1)
Vapor Pressure (VP)	1.09E-07 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.19
((C) 1994-2008 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

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